Environ 2001™ Software: Environmental, Safety and Health Property Data and Estimations for the 21st Century

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AIChE DIPPR® Project 911 has been developing a comprehensive database of physical properties for chemicals that are regulated by various agencies of the United States government, and are important to the chemical process industry. Project 911 collects and quantitatively reviews Environmental, Safety and Health (ESH) data for over 1000 chemicals and 56 physical properties. Physical properties within Project 911 include aqueous solubility, octanol-water partition coefficients, vapor pressure, aquatic toxicity, bioconcentration factor, flash point, and activity coefficients at infinite dilution. Estimation techniques and recommended physical property values from our database of over 140,000 data points are delivered to the user by a new Visual Basic™ software product, Environ 2001™, which is being sold commercially by EPCON International. Environ 2001™ uses traditional thermodynamic relationships, group contribution techniques such as UNIFAC and Hine and Mookerjee, and new algorithms developed at Michigan Technological University to estimate physical property data values where experimental data values are not available. The ultimate goal of Project 911 is to develop, thoroughly review, and deliver a high quality ESH database and additional estimation techniques that can be used to support engineering and regulatory calculations.